Co-Optimization of
Fuels & Engines

Overview

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Project # FT037

June 8, 2017

FY17 Vehicle Technologies Office
Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

VTO Program Managers: Gurpreet Singh , Kevin Stork, Leo Breton & Michael Weismiller

Goals and Outcomes

Light-duty

Boosted SI: Up to 15% fuel economy (FE) improvement beyond the projected results of current R&D efforts*

Multi-mode SI/ACI:
Up to 5% additional FE benefit beyond boosted SI

Heavy-duty

Up to 1-4% FE improvement (worth $1-5B/year)*

Potential lower cost path to meeting next tier of criteria emissions regulations

Fuels

Diversifying resource base

Providing economic options to fuel providers to accommodate changing global fuel demands

Providing market pull for up to 25 billion gallons/year of domestically sourced fuels

Cross-cutting goals

Maximizing impact on domestic economy

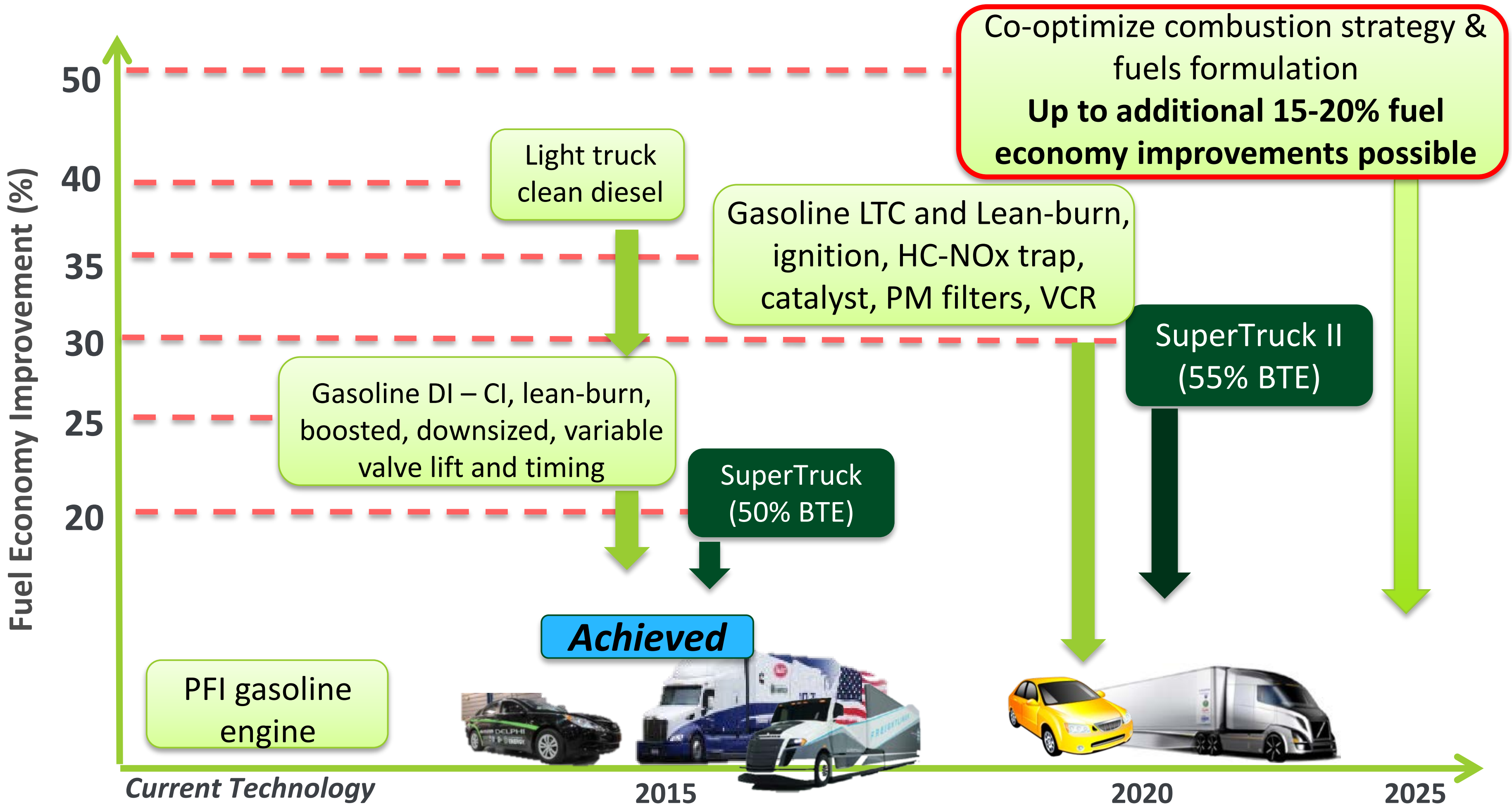
Adding up to 500,000 new jobs

Providing market-based approach for reducing emissions (GHG)

* The team is actively engaging with OEMs, fuel providers, and other key stakeholders to refine goals and approaches to measuring fuel economy improvements

Research Roadmap for 2015 and Beyond – *Addressing Critical Technical Barriers for Light- and Heavy-Duty Vehicles*

Increase Engine Efficiency to Improve Fuel Economy



Overview

Timeline

- Project start date: 10/1/2016
- Project end date:* 9/30/2018
- Percent complete: 56%

Budget

	FY16 Budget	FY17 Budget	FY18 Budget
VTO	$12,000	$12,500	$12,500
BETO	$14,000	$12,000	$12,000
Total	$26,000	$24,500	$24,500

* Start/end dates refer to three-year life cycle of DOE lab-call projects. Co-Optima is expected to be proposed for an additional three-year cycle at the end of FY18

Barriers

Inadequate data and predictive tools for:

- Fuel property effects on combustion and engine efficiency optimization
- Fuel effects on emissions and emission control system impacts
- Long-term impact of fuel and lubricants on engines and emission control systems

Partners

Partners include nine national labs, 13 universities, external advisory board, and stakeholders (129 individuals from 77 organizations)

Budget by Presentation

Topic	Presenter	FY16 ($K)	FY17 ($K)	FY18 ($K)
Overview	Farrell	1,000	1,000	1,000
Fuel property characterization and prediction	McCormick	1,300	1,300	1,300
Fuel property impacts on SI efficiency Part 1: RON, S, HOV	Szybist	1,400	1,300	1,300
Fuel property impacts on SI efficiency Part 2: Flame speed, LSPI, and merit function development	Kolodziej	1,200	1,300	1,300
Multimode Lean SI: Experiments and Simulation	Sjoberg	1,700	1,900	1,900
Exploratory advanced compression ignition combustion tasks	Dec	2,300	2,300	2,300
Emissions, Emission Control, and Sprays	Toops	1,600	1,800	1,800
Fuel kinetics and simulation tool development	McNenly	1,500	1,600	1,600
Total		12,000	12,500	12,500

Co-Optima Organization

Board of Directors
(Labs and DOE)
Approve direction and changes in focus

Steering Committee
POC for each lab, communications, IP

Operations
Project management, project integration, and strategic consulting

Leadership Team
(Labs and DOE)

Establish vision, define strategy, integrate work plan, oversee execution, evaluate performance, engage stake holders, and team build

External Advisory Board
Advise on technology and direction, provide recommendations, bridge to stakeholders

Technical Team Leads
Plan projects, evaluate team performance and gaps, report monthly highlights and quarterly progress, communicate across teams to minimize silos

Partners – External Advisory Board

USCAR
David Brooks

American Petroleum Institute
Bill Cannella

Fuels Institute
John Eichberger

Truck & Engine Manufacturers Assn
Roger Gault

Advanced Biofuels Association
Michael McAdams

Flint Hills Resources
Chris Pritchard

EPA
Paul Machiele

CA Air Resources Board
James Guthrie

UL
Edgar Wolff-Klammer

University Experts
Ralph Cavalieri (WSU, emeritus)
David Foster (U. Wisconsin, emeritus)

Industry Expert
John Wall (Cummins, retired)

- EAB advises National Lab Leadership Team
- Participants represent industry perspectives, not individual companies
- Entire board meets twice per year; smaller groups meet on targeted issues

Relevance

- Internal combustion engines will dominate the fleet for decades and their efficiency can be increased significantly
- Research into better integration of fuels and engines is critical to accelerating progress towards economic development, energy security, and emissions goals
- Improved understanding in several areas is critical for progress:
    - Fuel chemistry – property relationships
    - How to measure and predict fuel properties
    - The impact of fuel properties on engine performance
- Relevant to LD SI, MD/HD diesel, and ACI combustion strategies
- Addresses VTO program plan knowledge gaps surrounding advanced combustion engine regimes and predicting the impact of fuel properties

Overall Co-Optima Objectives

- Identify engine parameters and fuel properties that can significantly increase fuel economy across light, medium, and heavy duty fleets
  - Focus is on precompetitive, early TRL research
  - We are not looking to define or recommend commercial solutions
- Develop technical basis for new fuel specifications
- Conduct comprehensive and consistent survey of blendstock candidates to identify broad range of options that can be blended into petroleum base stocks and yield target values of key properties
- Identify blendstocks candidates that can be produced from renewable domestic feedstocks and offer technical and societal gains
- Identify implications to the refueling infrastructure for the various blendstock options
- Develop tools that allow us to do the work faster and more efficiently
- Identify options that provide “wins” for broad range of stakeholders

Milestones*

Month / Year	Description of Milestone or Go/No-Go Decision	Status
Dec 2016	Complete development of Thrust II strategy and deliver summary report document to DOE	Complete
Mar 2017	Release preliminary version of Co-Optimizer tool	Complete
Mar 2017	Go/no-go milestone	Complete
Jun 2017	Hold Decision Point review and document outcome of results	On track
Sep 2017	Complete market acceptance and implementation strategy for Thrust I fuel	On track
Sep 2018	Finalize technical basis for boosted SI fuel specification	On track

- Table reflects high-level "dashboard" milestones
- Overall effort has > 100 milestones
- Many milestones discussed in following presentations

Governing Hypotheses

Central Engine Hypothesis

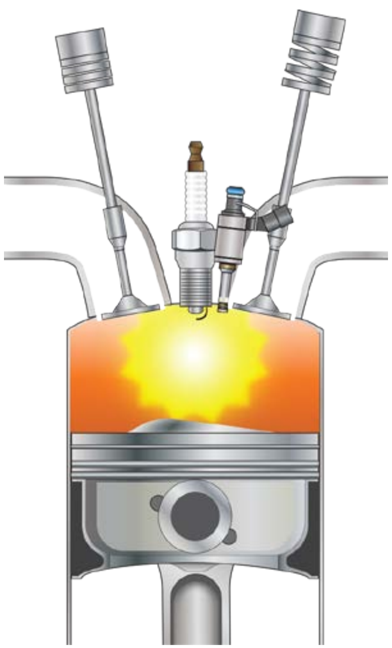
There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range

Central Fuel Hypothesis

If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance

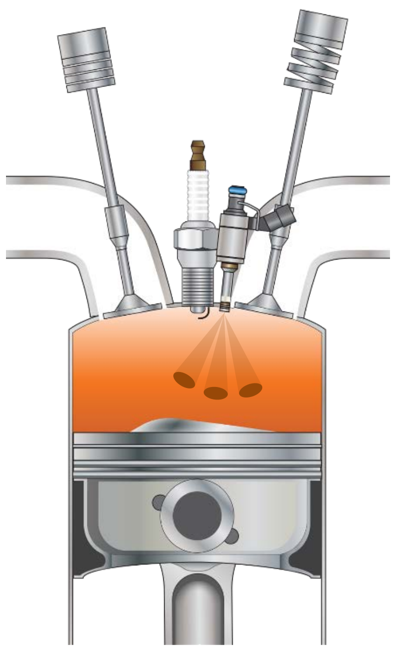
Two Parallel R&D Projects

Light-Duty



Boosted SI

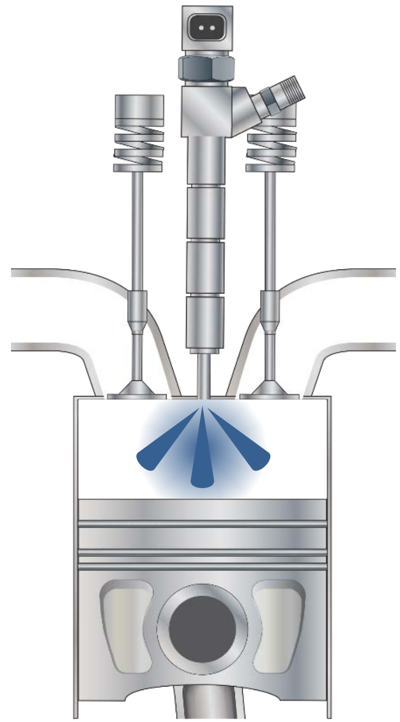
Near-term



Multi-mode SI / ACI

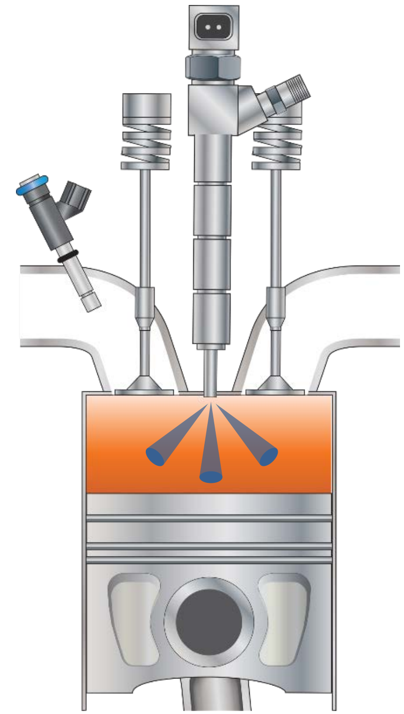
Longer-term

Medium and Heavy-Duty



Mixing Controlled

Near-term



Kinetically Controlled

Longer-term

Overview of approach

Co-Optima is focused on identifying fuel properties that optimize engine performance, <u>independent of composition</u>,* allowing the market to define the best means to blend and provide these fuels

* We are not going to recommend that <u>any</u> specific blendstocks be included in future fuels

New fuel specs would be analogous to today's gasoline spec, in contrast to (e.g.,) E85

However, in support of this, we are pursuing a systematic study of blendstocks to identify a broad range of feasible options

Objective is to identify blendstocks that can provide target ranges of key fuel properties, identify trade-offs on consistent and comprehensive basis, and share information with stakeholders

We are also looking to identify options that can be sourced from biomass while providing technical and societal benefits

Main elements of approach

- Identify key fuel properties that impact efficiency for advanced SI and CI combustion approaches
  - Utilize "efficiency merit function" to identify most important property impacts
  - Utilize final validated merit function as technical basis for fuel property specification
- Apply tiered approach to identify blendstock options that provide key fuel properties
  - Identify barriers to widespread commercial introduction
  - Focus on options with viable routes to near-term commercial use (petroleum- or bio-based)
  - Identify blendstocks that provide value when produced from biomass
- Identify ways to co-optimize, i.e., identify options that provide "wins" for broad range of stakeholders

Efficiency Merit Function Approach

- Research framed around "efficiency merit function" that estimates potential engine efficiency gains associated with changes in key fuel properties
  - The efficiency gains are not the same as fuel economy gains, which depend on both fuel (energy density) and vehicle (powertrain) design choices
- Merit function establishes fuel property relationships in a systematic and comprehensive way that guides R&D
- Each combustion approach (boosted SI, multimode ACI, etc.) will have it's own unique merit function
- Efforts underway to automate merit function to quantify uncertainty and identify experiments/simulations that will reduce uncertainties

Merit Function has been updated

$$Merit = \frac{(RON_{mix} - 91)}{1.6} - K\frac{(S_{mix} - 8)}{1.6}$$

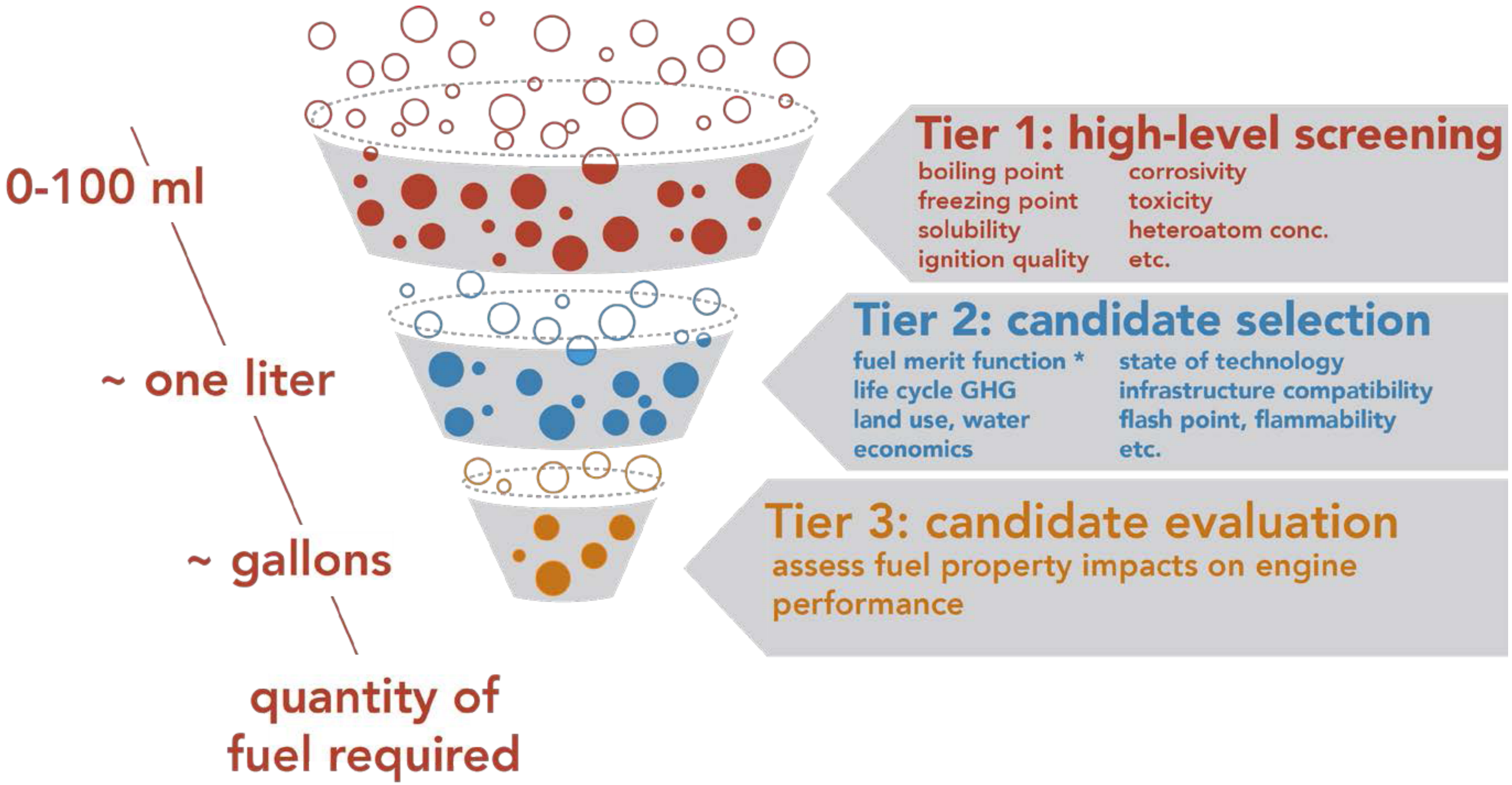
$$+\frac{0.085[ON/kJ/kg_{mix}]\cdot((HoV_{fuel}/(AFR_{stoich}+1)) - (415[kJ/kg_{fuel}]/(14.3[-]+1)))}{1.6}$$

$$+\frac{((HoV_{fuel}/(AFR_{stoich}+1)) - (415[kJ/kg_{fuel}]/(14.3[-]+1)))}{15.38} + \frac{(S_{Lmix} - 46[cm/s])}{5.4}$$

$$-H\left(PMI - 1.6\right)\left[0.7 + 0.5(PMI - 1.4)\right] + 0.008°C^{-1}\left(T_{c,90,conv} - T_{c,90,mix}\right)$$

- Major changes since last year:
  - Updated coefficients for RON, S, HoV, S_L, and PMI
  - Deletion of term for low-speed pre-ignition (LSPI)
  - Addition of term to reflect cold start

Tiered approach to blendstock screening, selection, and evaluation



- Tier 2/Tier 3 transition recently occurred at Decision Point review
- Eight representative blendstocks (of the 41 Tier 2 blendstocks) advanced to Tier 3 evaluation stage at 3/29/17 Decision Point review

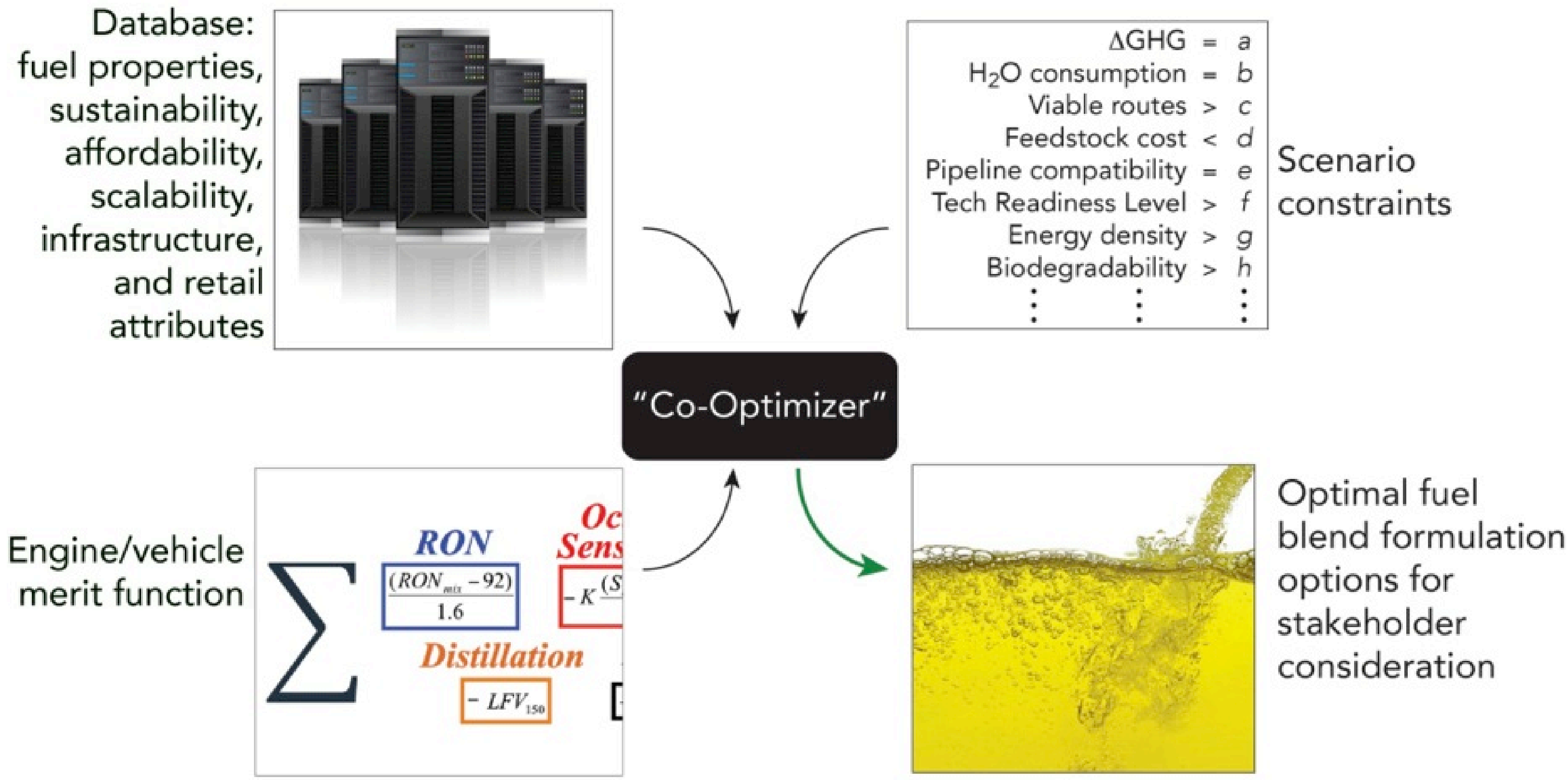
Assessing viability: 2025-2030 time frame

Technology Readiness	Environmental	Economics	Market
SOT - fuel production	Carbon efficiency	Target cost	Uncertainty
SOT - vehicle use	Target yield	Needed cost reduction	Regulatory requirements
Conversion TRL level	Life cycle GHG	Co-product economics	Geographic factors
Feedstock sensitivity	Life cycle water	Feedstock cost	Political factors
Process robustness	Life cycle FE use	Alternative high-value use	Vehicle compatibility
Feedstock quality			Infrastructure compatibility
# of viable pathways			

SOT = state of technology; TRL = technology readiness level; GHG = greenhouse gas; FE = fossil energy

- Twenty three metrics identified to assess feasibility of commercial introduction in 2025-2030 timeframe
- Technology readiness, environmental, and economic analyses restricted to bio-derived pathways (addresses gap in understanding)
- Market assessments apply to both petroleum- and bio-derived routes

Co-Optimizer – Approach and Tool



The Co-Optimizer computational tool will identify fuel formulations that meet commercial fuel specifications and maximize engine efficiency, subject to various constraints

Efforts underway to clarify value propositions for all major stakeholder groups (including consumers)

Goal is to identifying deployment scenarios with maximum market pull for all stake-holder groups (a "win" for all)

Go/No-Go Milestone

- Milestone: Demonstrate that two fuels with the same values of key fuel properties but different compositions provide equivalent engine performance (within experimental error) at a set of loads and speeds identified in consultation with external stakeholders
- The Go/No-Go Milestone Review is intended to
  - Demonstrate sufficient progress on R&D for boosted SI engines to justify continued funding
  - Establish validity of the research approach (e.g., Central Engine and Central Fuel Hypotheses)
  - Determine if the project scoped around the Central Hypotheses is able to lead to success.
- Go/No-Go Milestone Review held March 29, 2017; project received a "go."
- Details covered in later presentation ("Fuel Property Impacts on SI Engine Efficiency Part I")

Ten Major Accomplishments

1. Developed and tested Central Fuel Hypothesis
2. Constructed and updated LD boosted SI merit function
3. Refined understanding of how fuel properties affect engine combustion
4. Developed and populated fuel property database with 400+ blendstocks and fuel mixtures
5. Selected 40+ high-potential boosted SI blendstocks and identified 8 representative Tier 3 blendstocks
6. New insights into compatibility of boosted SI fuel properties with GCI strategies
7. Developed co-optimizer approach and methodology
8. Completed cost & environmental impact analyses (LCA, TEA) of 20 promising boosted SI candidates [1]
9. Completed benefits analysis (impact of Co-Optima) [1]
10. Maintained extensive external stakeholder engagement [1]

[1] Reflects work predominantly funded by BETO and not covered in today's AMR presentations

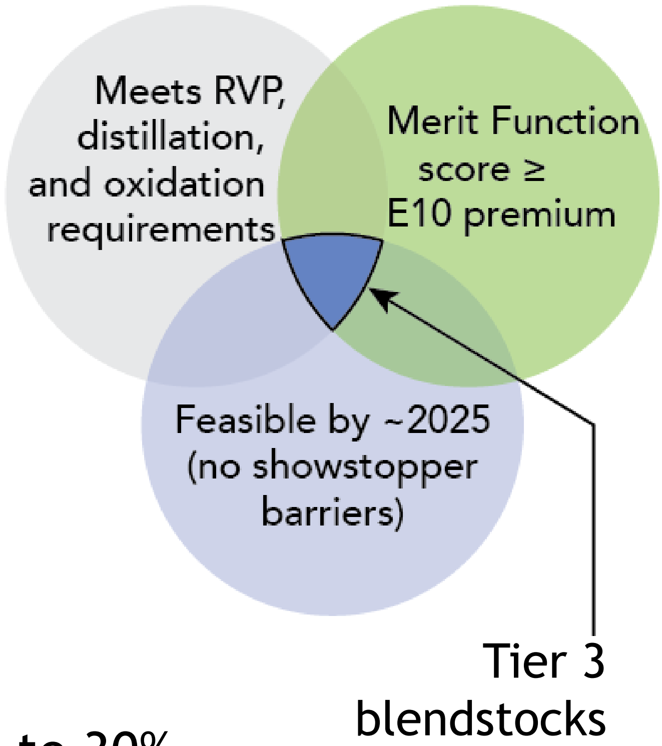
Decision Point Outcome

Decision point review held March 29, 2017

Purpose: identify which of the 41 Tier 2 blendstocks merit advancing to Tier 3 evaluation (see slide 18)

Criteria:

1. Meet current critical fuel requirements (RVP, distillation, oxidative stability, etc.) when blended in petroleum BOB
2. Achieve merit function score ≥ E10 premium when blended in petroleum BOB at levels up to 30%
3. No "showstopper" barriers (must have viable path to potential market introduction by ~2025-2030)



Eight representative candidates identified; future work will focus on experimental evaluations and identifying key barriers and research needs for each blendstock

Response to Previous Year Reviewers' Comments

- "… reviewer said the split between Thrust I and Thrust II is critical to maintain focus in the near-term and to not enter down a path of bias towards kinetically-controlled and compression ignition … also remarked that adding a decision point to extend the Thrust I program beyond 2019 would be beneficial."
  - As discussed previously, the structure and scope of the Co-Optima has evolved since the FY16 AMR to address this comment which has been raised by several stakeholders.
- "… reviewer suggested that it would behoove the Co-Optima panel to perform a thorough investigation to assess the use of the same fuel for both Thrust I and Thrust II engine concepts."
  - The Co-Optima research plan now includes the evaluation of Thrust I fuels with ACI concepts as well as a multimode advanced gasoline research topic which makes use of gasoline-like fuels with Boosted SI and ACI combustion.
- "… reviewer said that it looks like the project is just getting started and therefore there is not much progress yet on the project."
  - The Co-Optima initiative spans 9 national laboratories and two DOE offices so required considerable time to establish collaborations and an actionable research plan. The Co-Optima is now underway with many exciting accomplishments.
- "The reviewer did not like the fact that the first milestone is time driven and not event driven. The reviewer said that this time constraint could leave new developments out of the picture."
  - The LD project scope and time has been adjusted based on stakeholder input and is no longer targeted to conclude at the end of FY18

Remaining Challenges and Barriers

- Ensuring research pathways (e.g., boosted SI, ACI, etc.) have value for all stakeholders – this is critical for ensuring impact of this initiative on the introduction of better fuels and vehicles
- Further understanding of interdependencies of fuel properties and finalization of the merit function for advanced gasoline SI
- Understanding critical fuel properties for multimode SI-ACI combustion
- Identifying fuel properties critical for enabling higher engine system efficiency for ACI combustion
- Selecting high potential ACI combustion modes for the formation of multi-team research plans
- Maintaining strong stakeholder engagement

Collaboration/Coordination with Other Institutions

- Collaboration across nine national laboratories and two DOE offices
- Eight universities awarded up to $7M in FY17 FOA
  - Intent is to fully integrate university and national lab efforts
  - Kickoff meeting held April 28, 2017
  - Each team assigned a national lab “mentor” to facilitate integration and coordination
- Stakeholders (129 individuals from 77 organizations)
  - External advisory board (advising national labs, not DOE)
  - Monthly telecons with technical and programmatic updates
  - One-on-one meetings and conference presentations
  - Listening Days (three thus far)

Proposed Future Research

- Refine merit function development and establish technical basis for advanced gasoline fuel specification for boosted SI by end of FY18
- Initiate assessments and evaluations of eight Tier 3 representative candidates to
  - Provide critical information to industry/regulatory stakeholders
  - Provide foundation for development of fuel specification
  - Assess candidates for potential follow-on scale-up studies (outside Co-Optima)
- Expand advanced gasoline research to include multi-mode SI-ACI combustion
- Initiate multi-team ACI research for MD- and HD applications
- Develop approach (e.g., identification of critical fuel properties, merit function, fuel screening, simulation, etc.) for advanced gasoline multi-mode and ACI combustion platforms
- Continued strong engagement with stakeholders

Any proposed future work is subject to change based on funding levels

Much more detail will be presented in subsequent presentations

Summary

Relevance

- Better integration of fuels and engines research critical to accelerating progress towards economic development, energy security, and emissions goals

Approach

- Focused on identifying fuel properties that optimize engine performance, independent of composition, allowing the market to define the best means to blend and provide these fuels
- Leverages expertise and facilities from nine national laboratories and two DOE offices

Technical Accomplishments

- Major accomplishments span development of merit function, fuel database, new insight into fuel property impacts on engine efficiency, etc.
- Many additional accomplishments will be discussed in detail in subsequent presentations

Proposed Future Research

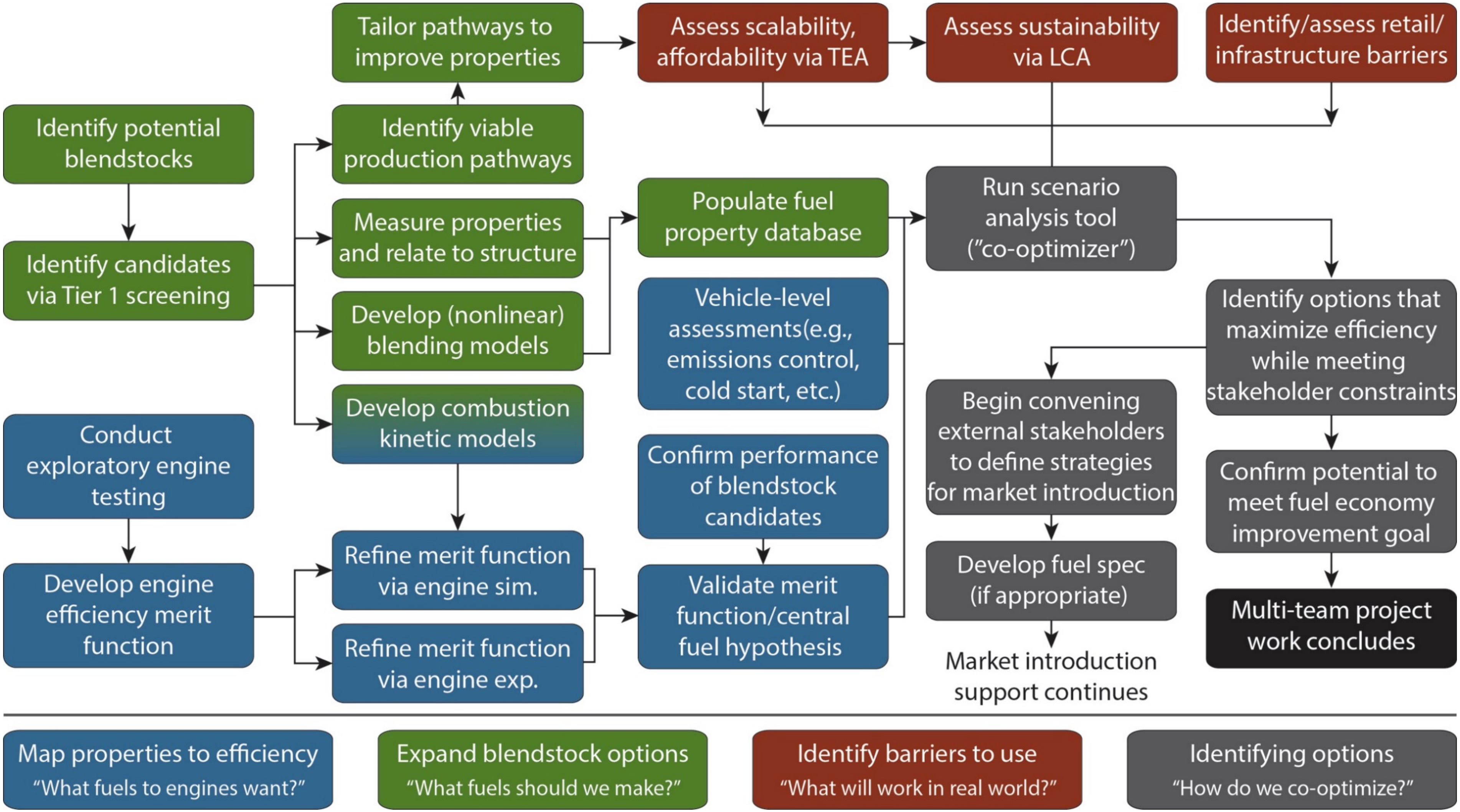
- Complete merit function development and establish fuel specification for boosted SI
- Expand advanced gasoline research to include multi-mode SI-ACI combustion
- Initiate more focused ACI research and approach for medium- and heavy-duty

Collaborations

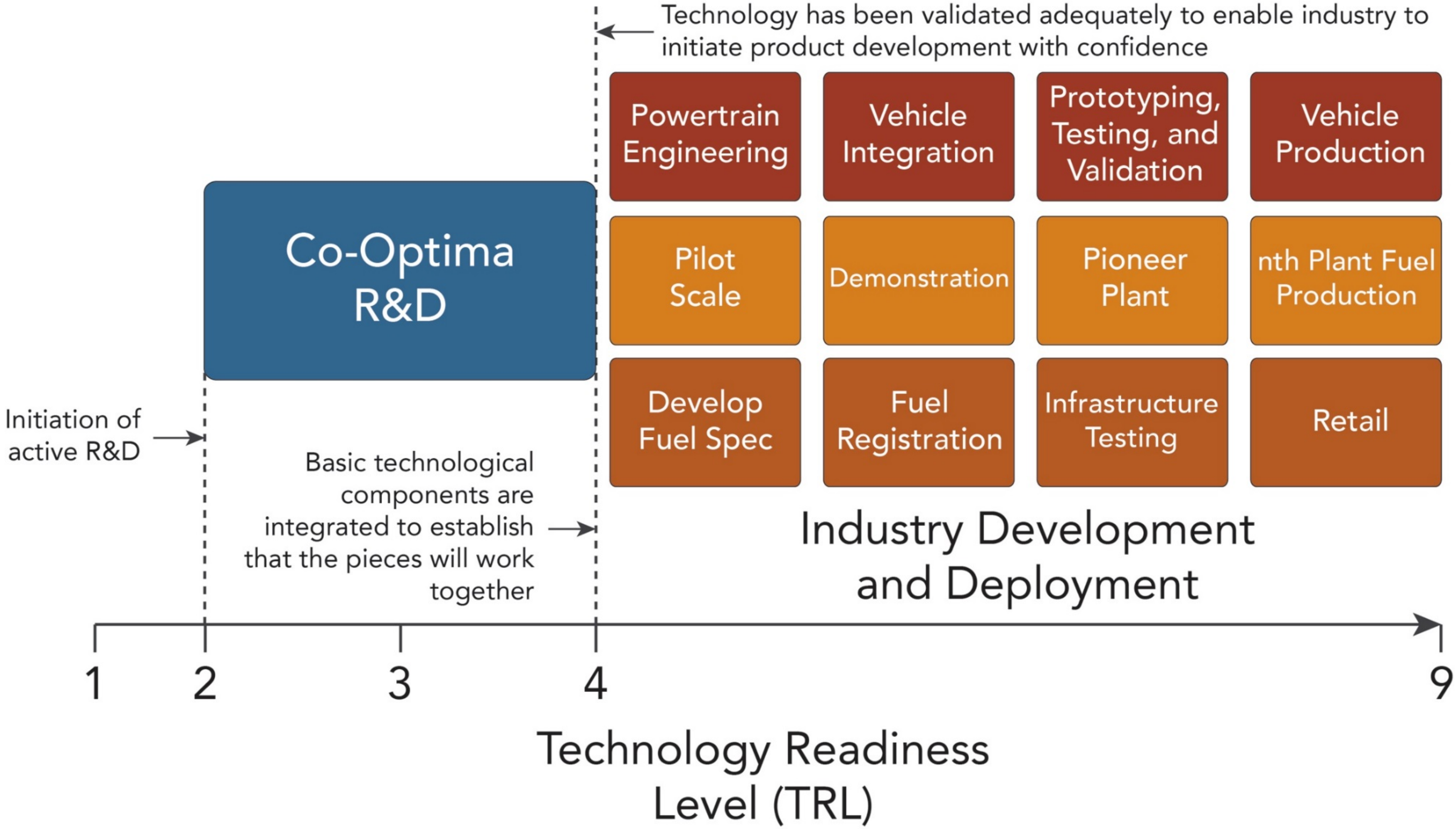
- Strong industry engagement including industry-led external advisory board, monthly stakeholder phone calls, and annual stakeholder meeting
- Collaboration across nine national laboratories, two DOE office, and thirteen universities

Technical Back-Up Slides

Technical Approach



Engagement with Industry



Partners – University Teams

1. Yale Univ./Penn State Univ.
   Measure sooting tendencies of various biofuels and develop emission indices
2. Univ. Michigan
   Engine combustion model simulating combustion duration, flame speed, and pressure development
3. Louisiana State Univ./Texas A&M/Univ. Connecticut
   Models and metrics for predicted engine performance
4. Univ. Alabama
   Combustion properties of biofuels and blends under realistic (ACI) engine conditions
5. Cornell University/UC San Diego
   Combustion characteristics of several diesel/biofuel blends
6. MIT/Univ. Central Florida
   Detailed kinetic models for several biofuels
7. Univ. Michigan-Dearborn/Oakland Univ.
   Miniature ignition screening rapid compression machine
8. Univ. Central Florida
   Measure and evaluate fuel spray atomization, flame topology, volatility, viscosity, soot/coking, and compatibility